

River Quality Modeling Using Differential Equations

Clark Bennett

University of South Dakota, cbennett@usd.edu

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Recommended Citation

Bennett, Clark (2001) "River Quality Modeling Using Differential Equations," *Rose-Hulman Undergraduate Mathematics Journal*: Vol. 2 : Iss. 1 , Article 1.

Available at: <https://scholar.rose-hulman.edu/rhumj/vol2/iss1/1>

River Quality Modeling Using Differential Equations

Abstract

A mathematical model provides the ability to predict the contaminant concentration levels of a river. The advection-diffusion equation is used as a first approximation for such a model. The validity of the model's results are compared with data gathered and compiled by the Minnesota Pollution Control Agency. A portion of the Mississippi River beginning at a site in the Southeast portion of Saint Paul, Minnesota and ending at a bridge near La Crosse, Wisconsin was used. The focus was to create the mathematical model and to compare its estimations against the available data on this portion of the river. Proceeding downstream, a river's contaminant concentrations can both increase and decrease due to factors such as tributaries, weather, and agricultural runoff. To fit the assumptions of a steady state advection-diffusion model, the contaminant concentration values that were utilized for the model were monotone increasing or decreasing above and below the tributary.

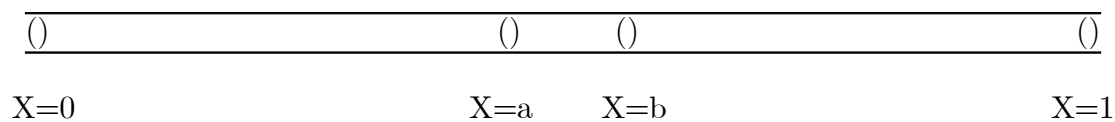
1. Introduction

1.1. Mathematical Modeling Information

This paper is on the development of a mathematical model that would be used for parameter identification and for the prediction of contamination levels along the river. The parameter of interest is to approximate the strength of any sources (or sinks) where the tributaries feed into the Missouri River. A source is when a tributary adds contaminants to the main body of the river and a sink implies that a tributary adds purer water to the main body of the river and therefore the contaminant concentration decreases.

1.2. Advection-Diffusion Equation History

For our model we assumed that the advection-diffusion equation may be a good first approximation to model the river contaminant levels. It was also assumed that the river had a uniform cross-sectional area. Therefore, the river was assumed to be linear or one-dimensional (a pipe with a uniform cross-sectional area).



A one-dimensional river cross-section with arbitrary interior and endpoints at $x=0$ and $x=1$.

The advection-diffusion equation in one dimension is given by

$$c_t = Dc_{xx} - Vc_x + f, \quad (1.1)$$

where the parameters are defined as follows: c is the concentration, x is the position on the river, t is the amount of time that passes, D is the diffusion factor, V is the velocity of the river, and f is the source or sink. A steady state solution is assumed, hence $c_t = 0$. The dimensions of the terms and coefficients in the equation are as follows: $c_t = [\frac{\text{concentration}}{T}]$, $c_x = [\frac{\text{concentration}}{L}]$, $c_{xx} = [\frac{\text{concentration}}{L^2}]$, $D = [\frac{L^2}{T}]$, $V = [\frac{L}{T}]$, and $f = [\frac{\text{concentration}}{T}]$. The derivation of equation (1.1) is as follows. The time rate of change in concentration amount of contaminants due to a tributary in the interval from point a to point b in the river is represented by

$$A \int_a^b f_o(x, t) dx, \quad (1.2)$$

where A is the cross-sectional area of the river and f_o is the source/sink. The total amount of contaminant in the river on the interval (a, b) , is given by

$$A \int_a^b c(x, t) dx. \quad (1.3)$$

The flux in concentration across a plane due to diffusion is the amount of concentration that passes through this plane due to the diffusion process. According to

Fick's Law of Diffusion, the concentration flux due to diffusion across any cross-section at a point a is proportional to the product of the cross-sectional area and the concentration gradient c_x . The flux in concentration due to diffusion at the points a and b with c_x being the concentration gradient is given by

$$-AD(a, c(a, t))c_x(a, t) \quad (1.4)$$

and

$$-AD(b, c(b, t))c_x(b, t) \quad (1.5)$$

respectively. The concentration flux due to advection across any cross-section at point x is proportional to the product of the velocity, cross-sectional area, and concentration. By conservation of mass we have

$$\begin{aligned} \text{time rate of change} &= \text{diffusion flux at (x = a)} - \\ \text{diffusion flux at (x = b)} &+ \text{advection flux at (x = a)} - \\ \text{advection flux at (x = b)} &+ \text{sources or sinks,} \end{aligned}$$

or equivalently,

$$\begin{aligned} \frac{d}{dt}A \int_a^b c dx &= -AD(a, c(a, t))c_x(a, t) + AD(b, c(b, t))c_x(b, t) \\ &+ VAc(a, t) - VAc(b, t) + \int_a^b f_o(x, t)dx. \end{aligned} \quad (1.6)$$

Now, divide through by A and let $((f_0/A) = f)$. Using the fundamental theorem of calculus,

$$\int_a^b \frac{d}{dx} f(x) dx = f(b) - f(a), \quad (1.7)$$

the result is

$$\int_a^b [(c)_t - (Dc_x)_x + (Vc)_x - f] dx = 0. \quad (1.8)$$

The choices of points a and b are arbitrary so the integral equation is written as the partial differential equation

$$c_t - (Dc_x)_x + (Vc)_x = f. \quad (1.9)$$

Assume that steady state holds ($c_t = 0$) and let D and V be constants so they can be pulled out of the x -partial derivative. The final equation appears as:

$$(0 = Dc_{xx} - Vc_x + f). \quad (1.10)$$

2. Experiment

2.1. Scaling the Modified Advection-Diffusion Equation

The advection-diffusion equation is used in modeling contaminant concentrations in ground water. The equation takes into consideration the following two processes: the change in concentrations due to diffusion (brownian motion, etc.) and the change in concentrations due to the velocity of the flow. The following equation and boundary conditions are used;

$$Dc'' - Vc' = -\alpha\delta(x - \xi), \quad (2.1)$$

$$c(0) = c_0, \quad (2.2)$$

and

$$c(1) = c_1, \quad (2.3)$$

where α is the strength of the source/sink ($\alpha > 0$ implies a source and $\alpha < 0$ implies a sink) due to the tributary at $x = \xi$. To scale equations (2.1)-(2.3) we let

$$\bar{c} = \frac{c * V}{\alpha}, \quad \bar{x} = \frac{x * V}{D}, \quad \bar{\xi} = \frac{\xi * V}{D}, \quad \bar{c}(0) = \frac{c_0 * V}{\alpha} = K_1, \quad \bar{c}(1) = \frac{c_1 * V}{\alpha} = K_2. \quad (2.4)$$

By the chain rule,

$$\frac{dc}{dx} = \frac{dc}{d\bar{c}} * \frac{d\bar{c}}{d\bar{x}} * \frac{d\bar{x}}{dx} = \frac{\alpha}{V} * \frac{d\bar{c}}{d\bar{x}} * \frac{V}{D} = \frac{\alpha}{D} * \frac{d\bar{c}}{d\bar{x}}. \quad (2.5)$$

Similarly,

$$\frac{d}{dx} = \frac{d}{d\bar{x}} * \frac{d\bar{x}}{dx} = \frac{V}{D} * \frac{d}{d\bar{x}}. \quad (2.6)$$

Therefore, equation (2.1) becomes

$$\frac{V * \alpha}{D} \bar{c}'' - \frac{V * \alpha}{D} \bar{c}' = -\alpha \delta\left(\frac{D}{V}(\bar{x} - \bar{\xi})\right) \quad (2.7)$$

where ($' = \frac{d}{d\bar{x}}$). By the properties of the Delta function, [Haberman (381-3)],

$$\delta(ax) = \frac{1}{|a|} \delta(x). \quad (2.8)$$

We can write the scaled, governing equation as the resulting second order,

non-homogeneous, differential equation

$$\bar{c}'' - \bar{c}' = -\delta(\bar{x} - \bar{\xi}). \quad (2.9)$$

Dropping the bars for convenience, the scaled equation takes on the form

$$c'' - c' = -\delta(x - \xi) \quad (2.10)$$

2.2. Derivation of the Solution

The Green's function method for the derivation of the solution to equation (2.10) is used.

Since $\delta(x, \xi) = 0$ for $x \neq \xi$, we solve the homogeneous equation

$$c'' - c' = 0. \quad (2.11)$$

The characteristic equation is

$$r^2 - r = 0. \quad (2.12)$$

Hence, the general solution and boundary conditions are:

$$c(x) = \begin{cases} A + Be^x & x < \xi \\ E + Fe^x & x > \xi \end{cases}, \quad (2.13)$$

$$c(0) = K_1, \quad (2.14)$$

$$c(1) = K_2. \quad (2.15)$$

For the purposes of maintaining continuity,

$$\lim_{x \rightarrow \xi^-} c(x) = \lim_{x \rightarrow \xi^+} c(x). \quad (2.16)$$

Applying the jump condition at $(x = \xi)$,

$$\int_{\xi-\varepsilon}^{\xi+\varepsilon} (c'' - c') dx = - \int_{\xi-\varepsilon}^{\xi+\varepsilon} \delta(x - \xi) dx. \quad (2.17)$$

Using properties of Green's function and the fundamental theorem of calculus gives

$$c'(\xi + \varepsilon) - c'(\xi - \varepsilon) - c(\xi + \varepsilon) + c(\xi - \varepsilon) = -1. \quad (2.18)$$

Taking $(\varepsilon \rightarrow 0)$, we get

$$c'(\xi^+) - c'(\xi^-) - c(\xi^+) + c(\xi^-) = -1. \quad (2.19)$$

Equations (2.14), (2.15), (2.16), and (2.19) are used to determine the four unknowns: A , B , E , and F .

Applying the boundary conditions (2.14) and (2.15) yields

$$K_1 = A + B; \quad (2.20)$$

$$K_2 = E + Fe. \quad (2.21)$$

Applying continuity at $(x = \xi)$ in (2.13) gives

$$A + Be^\xi = E + Fe^\xi. \quad (2.22)$$

Applying the jump condition and the continuity condition we get

$$Fe^\xi - Be^\xi = -1. \quad (2.23)$$

The resulting four equations and four unknowns yield

$$F = \frac{-1 + K_1e^\xi - K_2e^\xi + e^\xi}{e^\xi - e^{\xi+1}}, \quad (2.24)$$

$$E = K_2 - \left(\frac{-e + K_1e^{\xi+1} - K_2e^{\xi+1} + e^{\xi+1}}{e^\xi - e^{\xi+1}} \right), \quad (2.25)$$

$$A = K_2 - 1 - \left(\frac{-e + K_1e^{\xi+1} - K_2e^{\xi+1} + e^{\xi+1}}{e^\xi - e^{\xi+1}} \right), \quad (2.26)$$

and

$$B = K_1 - K_2 + 1 + \left(\frac{-e + K_1 e^{\xi+1} - K_2 e^{\xi+1} + e^{\xi+1}}{e^{\xi} - e^{\xi+1}} \right). \quad (2.27)$$

The resulting scaled concentration is given by,

$$c = \begin{cases} K_2 - 1 - \left(\frac{-e + K_1 e^{\xi+1} - K_2 e^{\xi+1} + e^{\xi+1}}{e^{\xi} - e^{\xi+1}} \right) + K_1 e^x \\ -K_2 e^x + e^x + e^x \left(\frac{-e + K_1 e^{\xi+1} - K_2 e^{\xi+1} + e^{\xi+1}}{e^{\xi} - e^{\xi+1}} \right) & x < \xi \\ \\ K_2 - \left(\frac{-e + K_1 e^{\xi+1} - K_2 e^{\xi+1} + e^{\xi+1}}{e^{\xi} - e^{\xi+1}} \right) \\ + e^x \left(\frac{-1 + K_1 e^{\xi} - K_2 e^{\xi} + e^{\xi}}{e^{\xi} - e^{\xi+1}} \right) & x > \xi \end{cases}. \quad (2.28)$$

2.3. Professional River Testing Data Information

The Minnesota Pollution Control Agency (MPCA) gathered data professionally on the upper Mississippi River in 1994. I tested my mathematical model with the advection-diffusion equation against this professionally gathered data. The Minnesota Pollution Control Agency had six testing sites on the upper Mississippi River where a major tributary existed between the first and second groups of three testing sites. The six testing sites are labeled (going from North to South): UM-840, UM-826, UM-815, UM-738, UM-714, and UM-698. The six testing sites

are located on the Minnesota Milestone Sites map in Appendix 1.

3. Results and Discussion

There are six sites I utilized from the Minnesota Pollution Control Agency (MPCA) along the upper Mississippi River. The data that I utilized had characteristics that fit the assumption for the model. The assumption was that the contaminant concentration was at steady state (concentration is independent of time). By differentiating equation (2.28) which is the solution with this underlying assumption, it can be shown that the concentrations must be monotone above and below the tributary. The use of the steady state assumption makes the problem easier to solve analytically and it is reasonable to assume that the contamination concentrations are not changing on a small time scale. The results of the model would not hold if the equilibrium is lost. The testing results were from the Total Solids and the Nitrates & Nitrites that were both measured in (mg/l). The major source that enters the Mississippi River is the St. Croix River, that enters just below site number three or UM-815 (see Appendix 1). This was the source/sink whose strength that was approximated. The total number of miles between sites one and six (UM-840 and UM-698) is 131 miles. The actual contaminant concentration values that I used in the six testing locations are located in Appendix

2. The scaled locations of each site as given by equation (2.4) is then: 0 for site one (UM-840), 0.092 for site two (UM-826), 0.191 for site three (UM-815), 0.206 for the source (the St. Croix River), 0.687 for site four (UM-738), 0.863 for site five (UM-714), and 1 for site six (UM-698). Appendices 3-6 are graphs showing the contaminant concentrations along the river. Equation (2.28) was used in conjunction with \bar{c} in equation (2.4) in order to determine the parameter $\frac{\alpha}{V}$. From equation (2.4), $\frac{\alpha}{V} = \frac{c}{\bar{c}}$ where c is the actual river contaminant concentration and \bar{c} is the scaled contaminant concentration as predicted by the model. For each of the four interior points, a $\frac{\alpha}{V}$ -value is obtained by looking at the quotient of c and \bar{c} . The average of these four $\frac{\alpha}{V}$ -values was used when estimating the river contaminant concentrations by the equation

$$c = \frac{\alpha}{V} * \bar{c}, \quad (3.1)$$

where the \bar{c} above is given by (2.28). Prior knowledge of V allows one to determine the source/sink parameter α by the product $\alpha = V * \frac{c}{\bar{c}}$. The $\frac{\alpha}{V}$ -values located in Appendix 7 can be thought of as an indicator of whether a cross-section of the river system with a tributary entering it is either a source or a sink ($\frac{\alpha}{V} > 0$ indicates a source and $\frac{\alpha}{V} < 0$ indicates a sink). The calculated concentrations placed in Appendix 7 originated from the math model prediction (2.28) with boundary

conditions. The average of the $\frac{\alpha}{V}$ -values calculated from the four interior points was then used to compare the contaminant concentration values predicted by the model against the actual concentration values for the interior four testing sites. The boundary points are not used for comparison since they match up for any $\frac{\alpha}{V}$ -value due to the boundary conditions of the problem. In Appendices 3-6, the actual and calculated values for the four interior testing points are plotted against each other for each month and test. The average percent error of the tests indicate that the model may have some validity. The Total Solids average percent error for April of 1994 is 7.94%. The Nitrates & Nitrites average percent error for May of 1994 is 4.56%. The Nitrates & Nitrites average percent error for June of 1994 is 12.23%. The Total Solids average percent error for September of 1994 is 47.05%.

4. Conclusions

Appendix 7 illustrates that all of the average $\frac{\alpha}{V}$ -values with the exception of two are negative. On the basis of this information, the St. Croix River tributary is classified as a sink. Since the average percent error values between the actual concentrations and the predicted concentrations using the model for April, May, and June of 1994 are less than 15.00%, it is concluded overall that the advection-

diffusion equation model was very effective in these particular examples. Since the Total Solids actual and predicted model concentrations for September of 1994 had an average percent error of 47.05%, one may hypothesize that this group of data had several collection inaccuracies or something else happened this month that the assumptions of the model were not satisfied. Two of the three remaining data groups, Total Solids of April of 1994 and Nitrates & Nitrites of May of 1994 closely matched the graphs of the actual values, while the last data group Nitrates & Nitrites of June of 1994 closely matched half of the actual data values. Although several assumptions were made early on in the problem, the modified advection-diffusion model shows considerable accuracy in predicting river contaminant levels.

5. Acknowledgments

I would like to say thank you to the Minnesota Pollution Control Agency (MPCA), Dr. Dan Van Peurse, Dr. Clayton Lehmann, Dr. Royce Engstrom, and Dr. Raymond Ring for all of their suggestions for this paper.

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